

Could anyone comment on any recent calculated results on the planarity, or lack thereof, of azobenzene?

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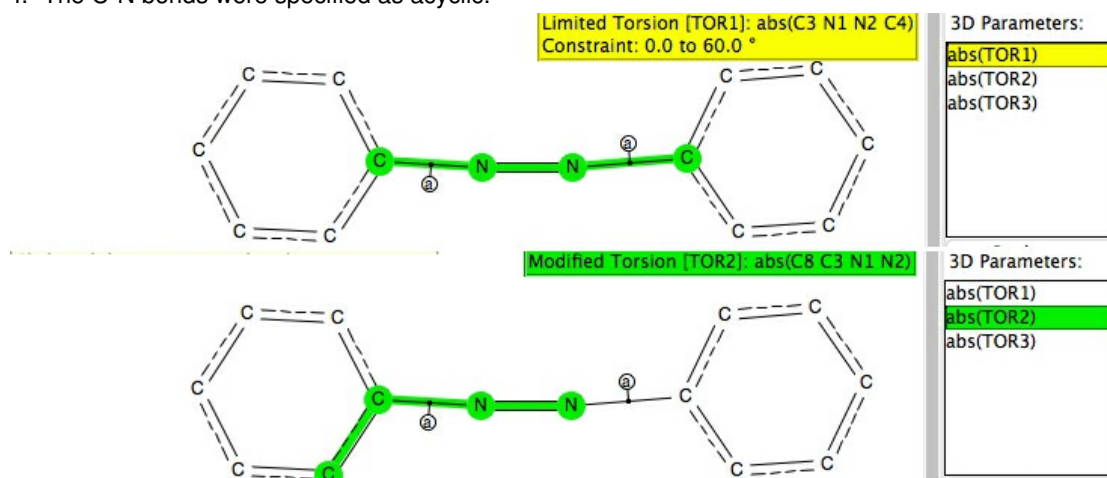
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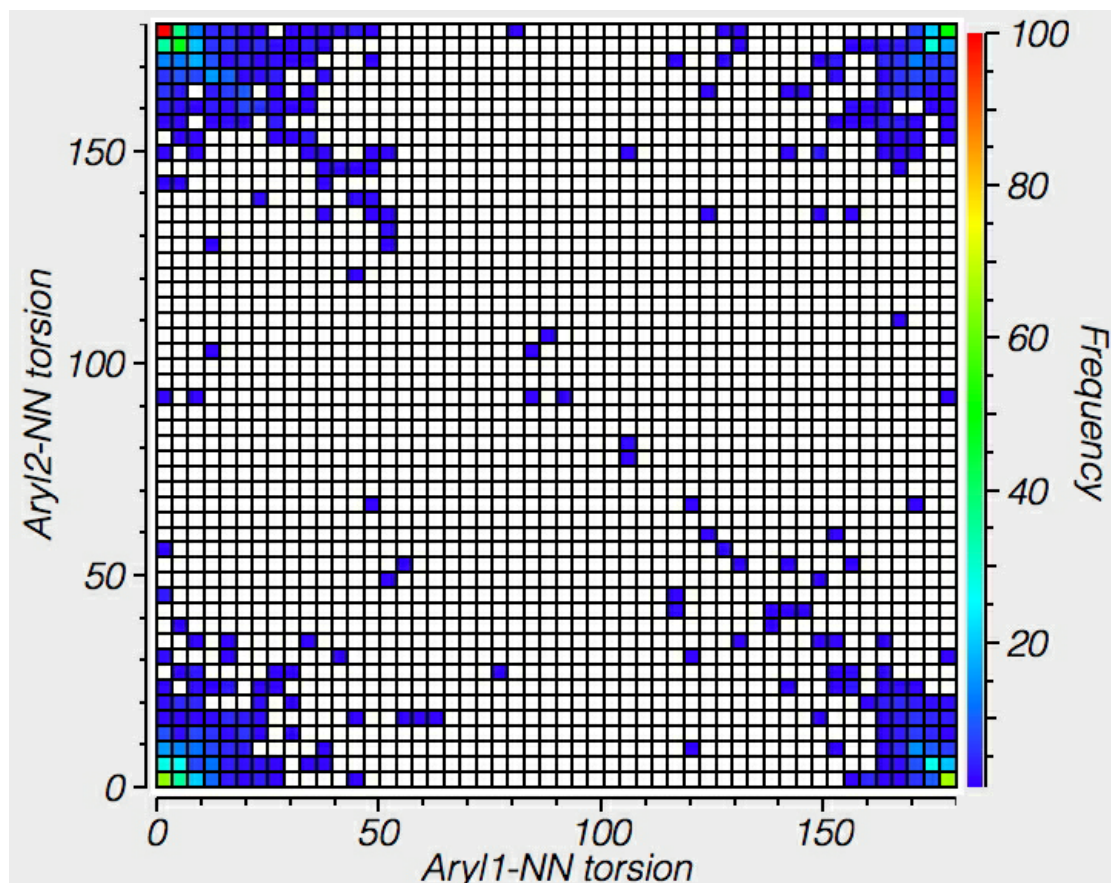
This question was [posted](#) on the [CCL](#) (computational chemistry list) by John McKelvey. Here, I give an answer in the form of a search of the CSD (crystal structure database).

I was not sure if the question related purely to the geometries obtained using computational methods or to comparisons with experimentally determined structures. Or indeed whether it related to azobenzene specifically or to azobenzenes in general. Here, I comment only in respect of the latter two. The search was defined as below, with the following specifications:

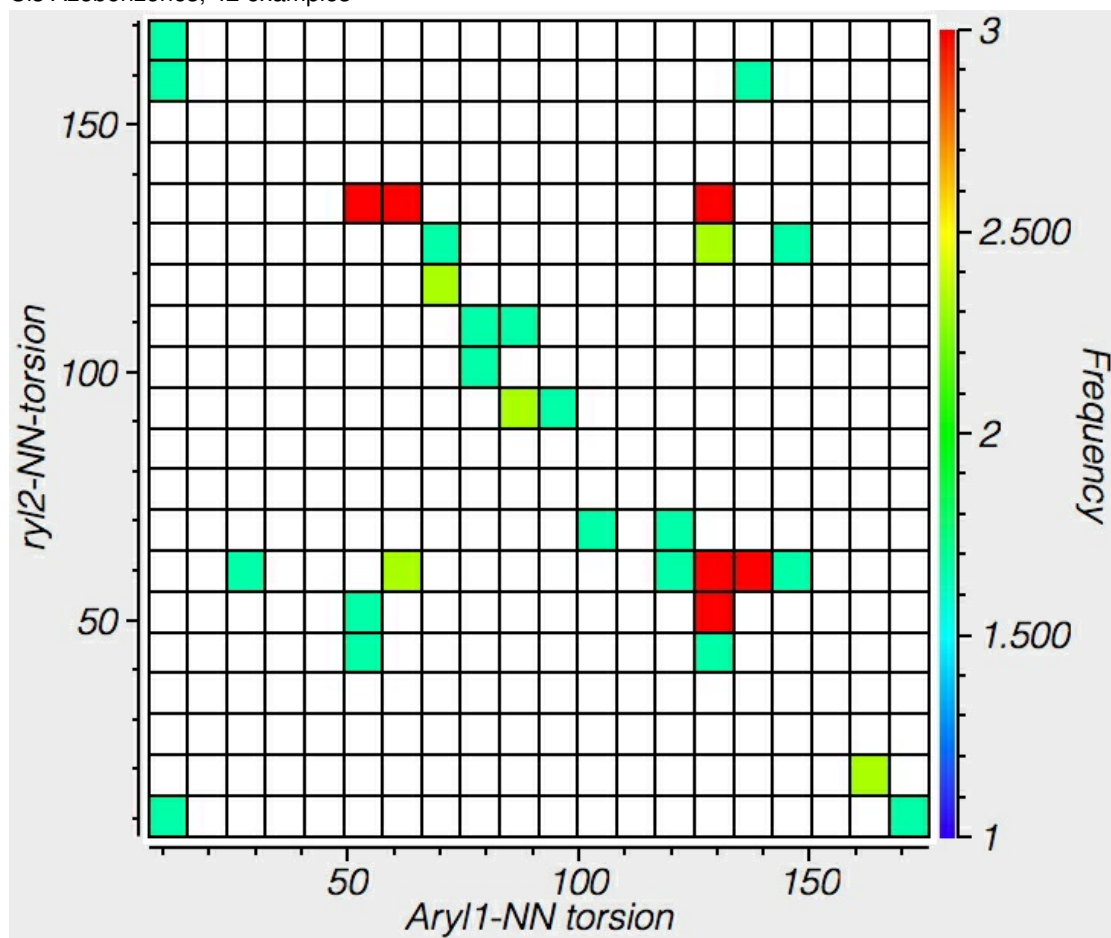
1. The absolute value of the central torsion (TOR1) was constrained to 0-60° for cis azobenzenes and to 120-180° for trans azobenzenes.
2. Two further torsions (TOR2, TOR3) specify the torsion angle about the aryl to N bond.
3. The R factor is < 0.1, and there are no errors or disorder.
4. The C-N bonds were specified as acyclic.



Trans Azobenzenes, 1111 examples



Cis Azobenzenes, 42 examples



The results show that by and large, trans azo-benzenes are co-planar to  $\pm 30^\circ$ , but there are some interesting points in the centre with dihedral angles of  $\sim 90^\circ$ . Cis azobenzenes on the other hand are mostly NOT planar, with red hotspots at about 50 or  $130^\circ$  of twist.

These results took about 20 minutes to define, search, and plot as per above. I hope it provides John with [an answer](#), even if it's not the one he might have meant!

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